Molecular dynamics modeling of particle and molecule interaction with solid and liquid surfaces

J.P. Allain, D.A. Alman,
M. Nieto, M.D. Coventry, Hua-Tan Qiu
and D.N. Ruzic

University of Illinois, Urbana-Champaign
Department of Nuclear, Plasma and Radiological Engineering

Plasma-Material Interaction Group

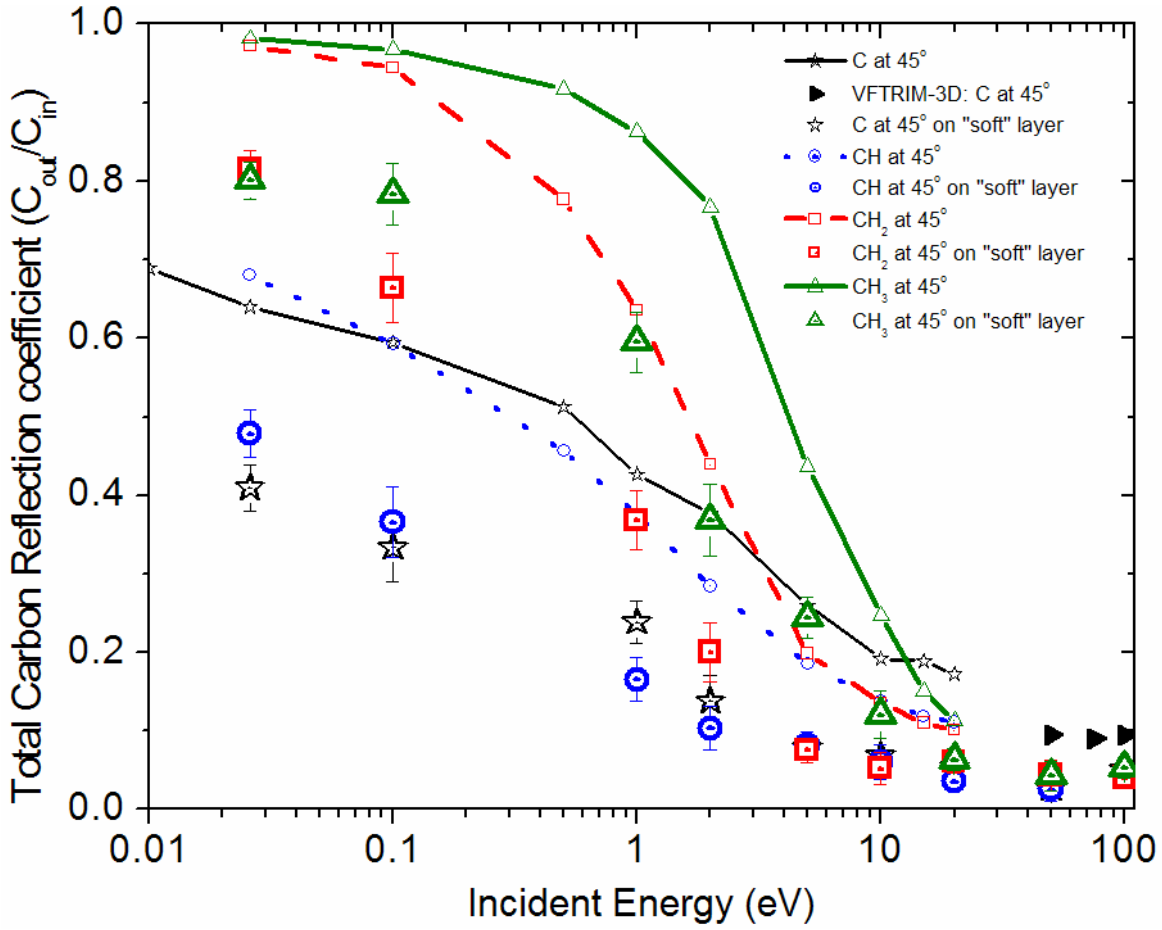
ALPS Meeting, Grand Canyon, AZ
April 9-11, 2003

Outline of Work at the UIUC

- Molecular Dynamics simulations of hydrocarbon plasma-material interaction
- Molecular Dynamics simulations of liquid lithium to study self-bombardment reflection
- Analytical studies of backscattered and sputtered charge fraction at low energies
- Liquid lithium erosion enhancement studies implementing a cascade model from molecular dynamics in a modified version of VFTRIM-3D
- Recent progress with FIRE first wall Be transport and divertor mixing issues

MD Modeling of Hydrocarbons

- First surface used was graphite bombarded by hydrogen until saturation (~ 0.4 H:C)
- Second surface - a “soft” H:C surface
  - Formed by deposition of thousands of hydrocarbons on a graphite surface
  - Emulates a redeposited carbon layer in a tokamak
    - Larger H:C ratio in this redeposited layer
    - Lower density
    - Carbon is less strongly bound
- Results show reflection is lower on the “soft” surface than the 0.4 H:C graphite at one energy (1 eV)
- Work continues to look at a full range of incident energies



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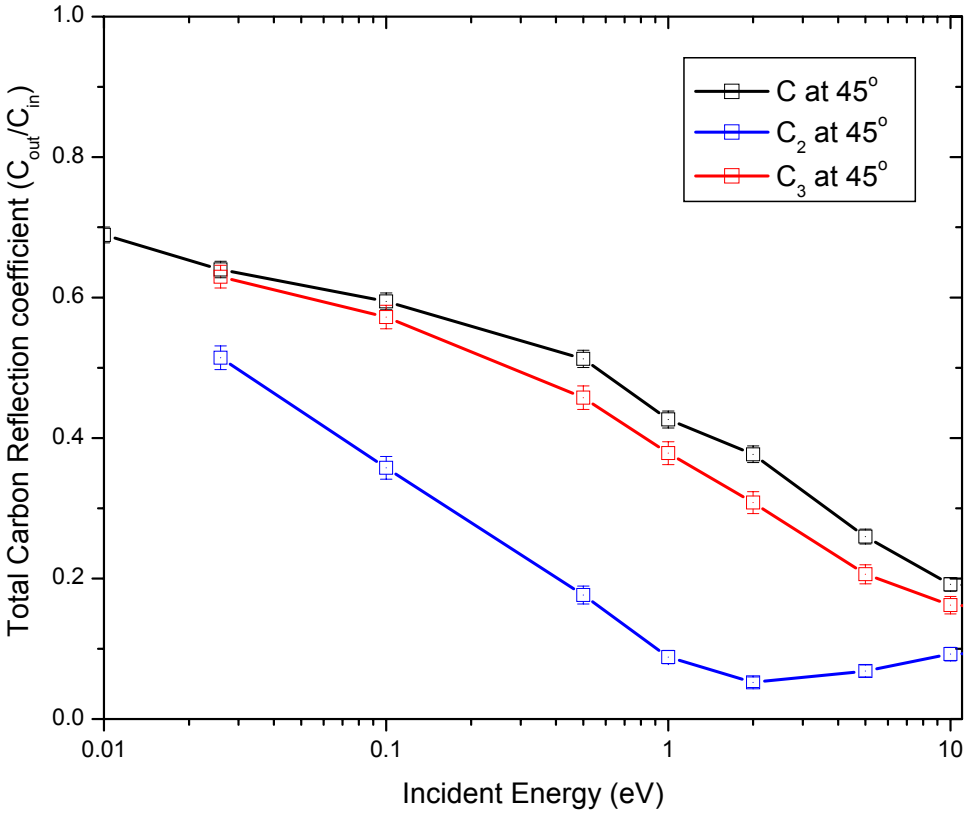
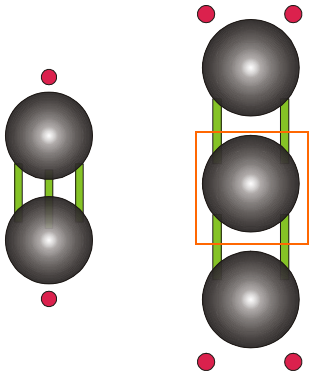
Reflection from “soft” vs. “hard” surfaces

- Why is reflection lower on the “soft” surface
  - The top layer of the “soft” surface is less dense
  - Incident atoms/molecules can penetrate more easily
  - Once inside the surface, the particles are more likely to be trapped there
  - On the “hard” surface, incident particles are more apt to have a hard collision on the very top surface and bounce off
  - Observation of more movies may provide further insight

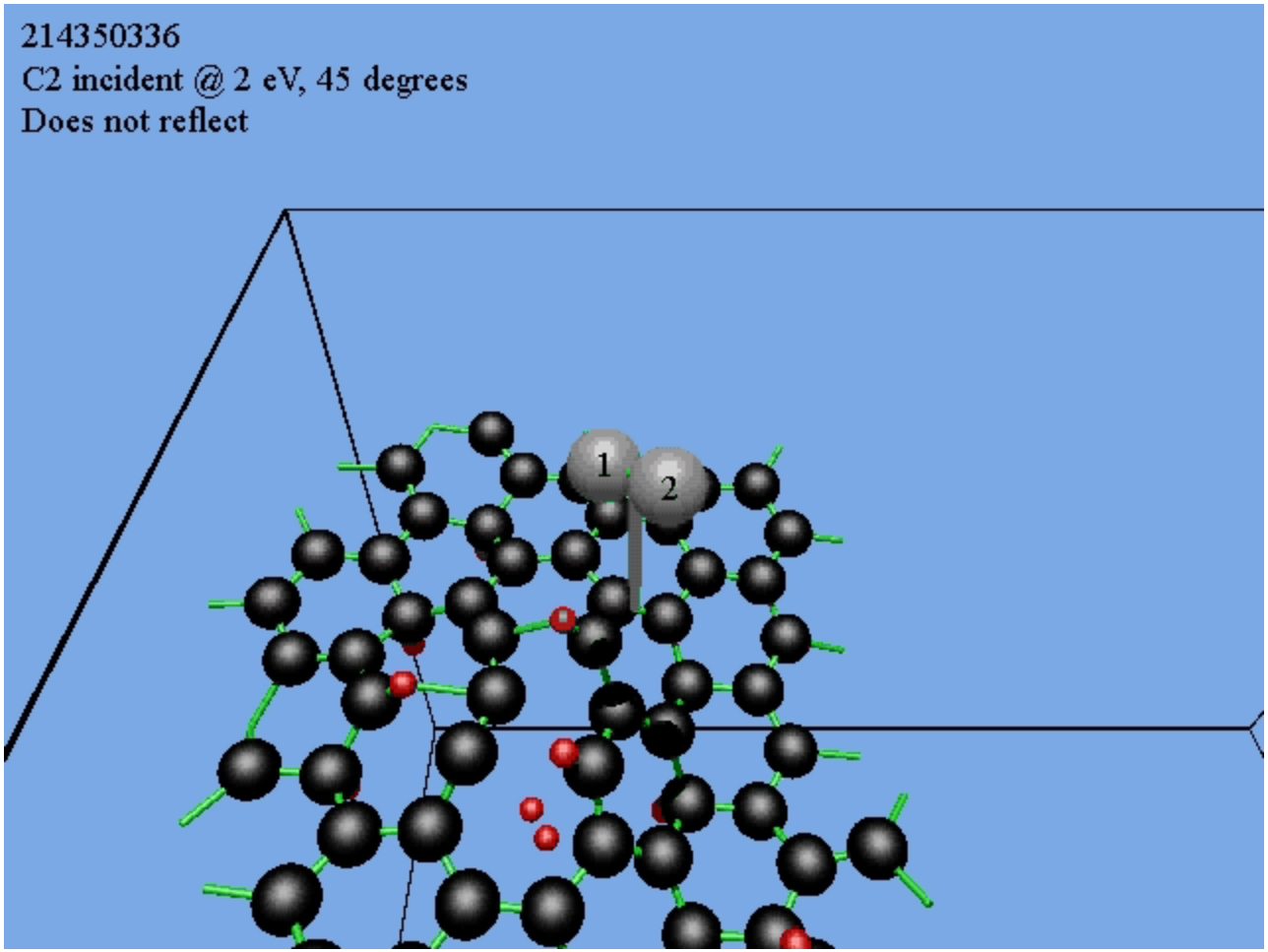
Reflection of carbon dimer and trimer molecules



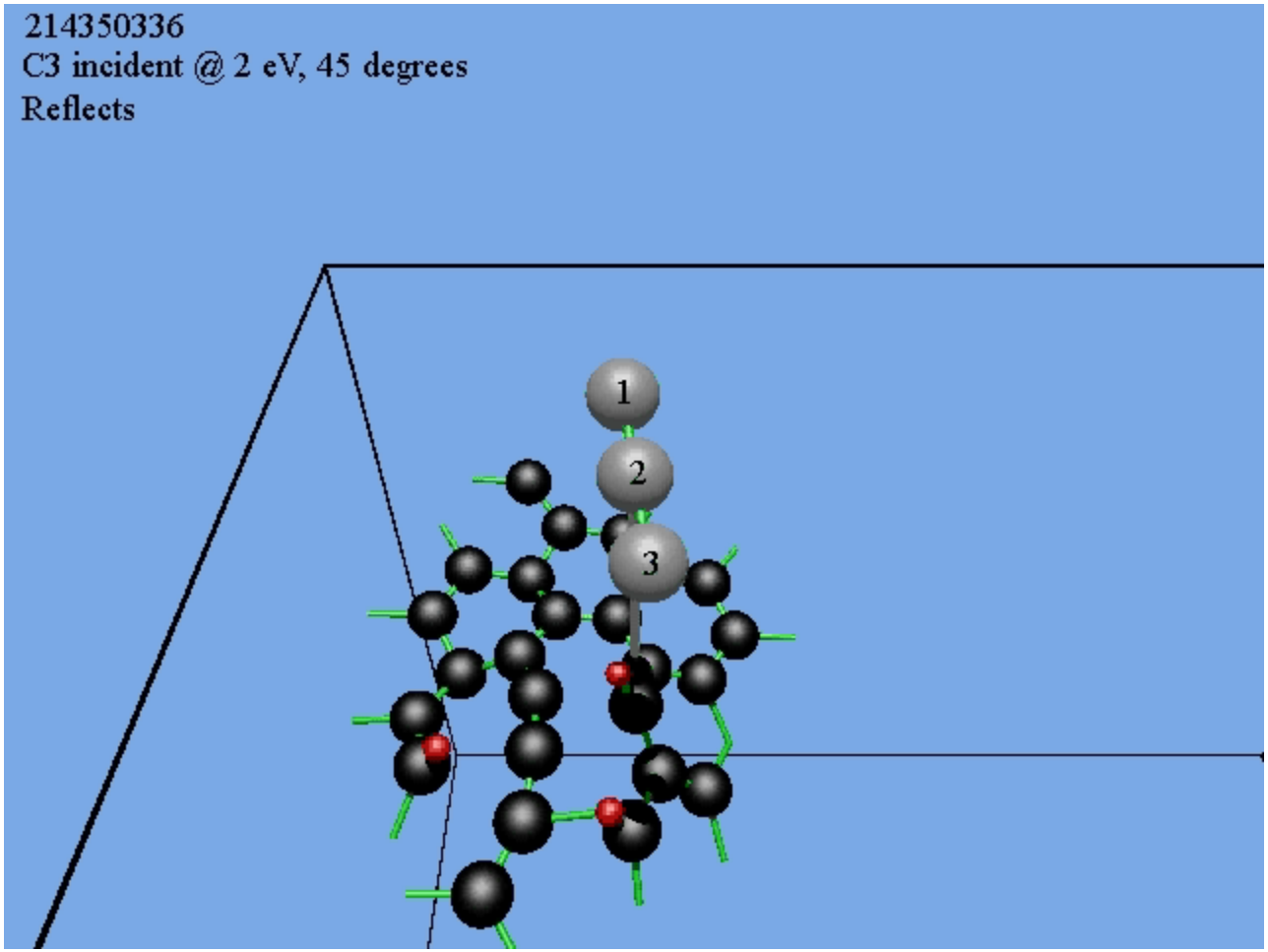
- Why does C_2 stick more readily than C_3?
  - One reason could be the fully bonded atom at the center of the trimer molecule
  - The end atom may attempt to stick, but when the molecule swings into position a repulsive force is created



Carbon dimer molecules tend to stick readily



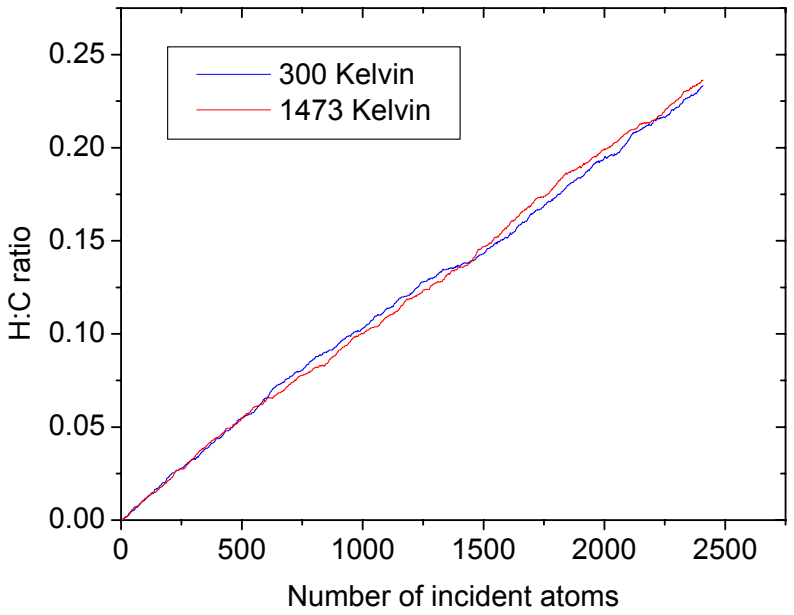
Carbon trimers are more likely to bounce off



Multi-scale problems: long time scale issues

- For example, does the graphite surface saturate at a lower H:C ratio at higher temperature?
- First attempt showed no difference between hydrogen concentration during H bombardment at room temp. & 1200 °C
- Possible issues:
  - Timescale for desorption of hydrogen is long ~10^{-6}-10^{-4} s
  - These MD simulations (e.g. to look at reflection) typically run for 10^{-13}-10^{-12} s
- Recent progress
  - Implemented a variable timestep algorithm in the MD code
  - Factor of ~3 speedup vs. fixed timestep with comparable accuracy

First attempt



- Enabled a long (100 ps) run to look at H desorption from the H saturated graphite surface
- Hydrogen is visibly more mobile
- 41% more H evolved at higher T, but still not conclusive

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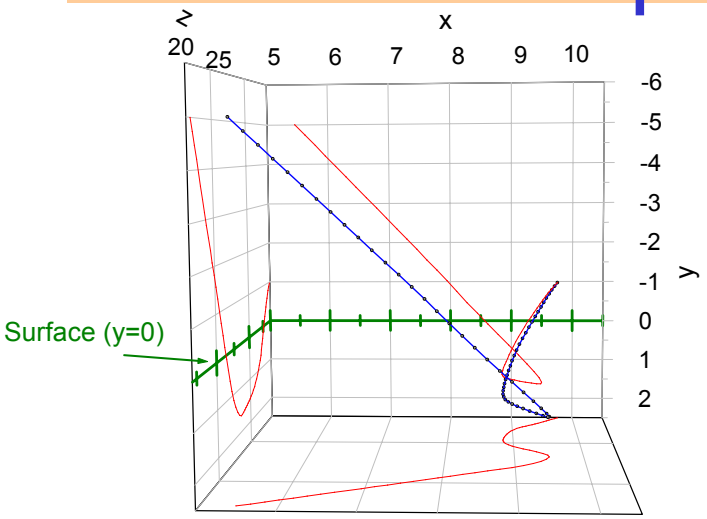
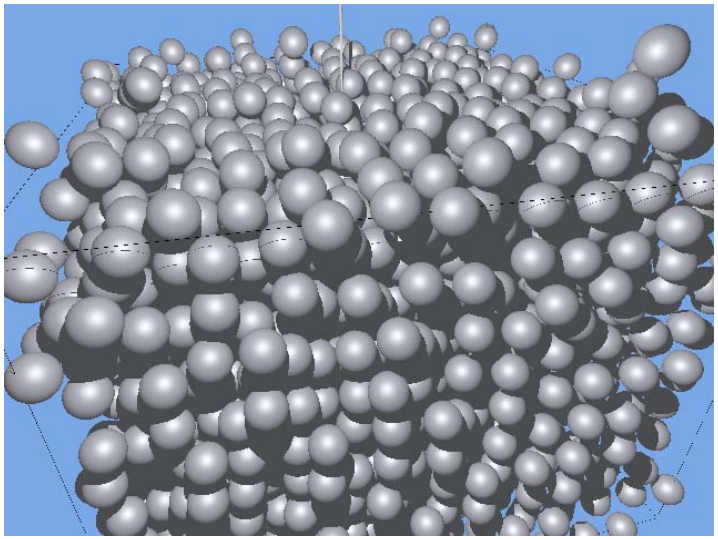
Modeling of reflection and charge state of backscattered particles

- Sputtered lithium particles in the ionized state leave surface at about 1-5 eV and quickly return to surface due to the magnetic sheath potential. Need to determine backscattering of incident lithium ions.
- Semi-analytical models exist to determine the charge state of backscattered particles from alkali metals such as lithium.

MD modeling of lithium bombardment on liquid lithium surfaces





- Investigation of reflection of lithium atoms on liquid lithium surfaces continues for NSTX conditions
  - 0.35 and 2 eV incident energy
  - 20 degrees incident angle
  - 473 K and 653 K surface temperatures
- Major changes have been made to the code to better incorporate lithium
  - Enabling lithium runs to be integrated into the distributed computing system already in use for hydrocarbon modeling (giving ~10x speed-up)
  - Calculation of ion fraction of reflected/sputtered atoms now built in
  - New liquid lithium potential data included†

† L.E. Gonzalez, private comm. 2002 Universidad de Valladolid

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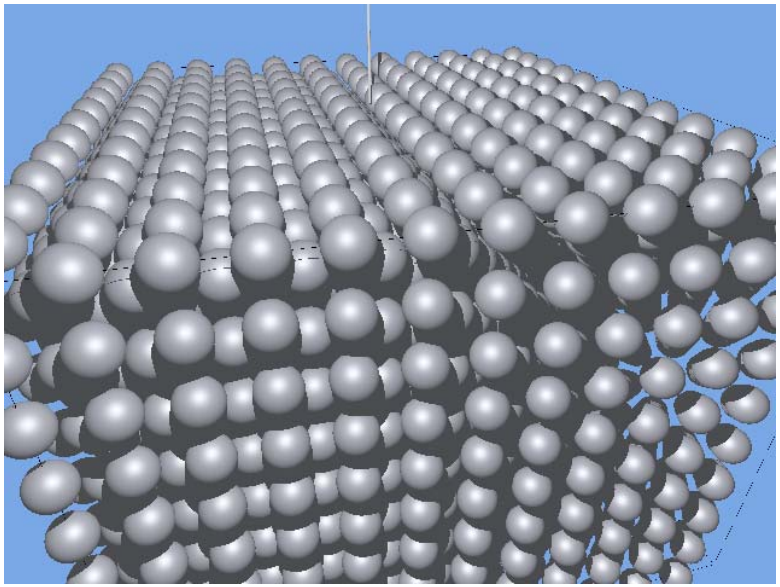
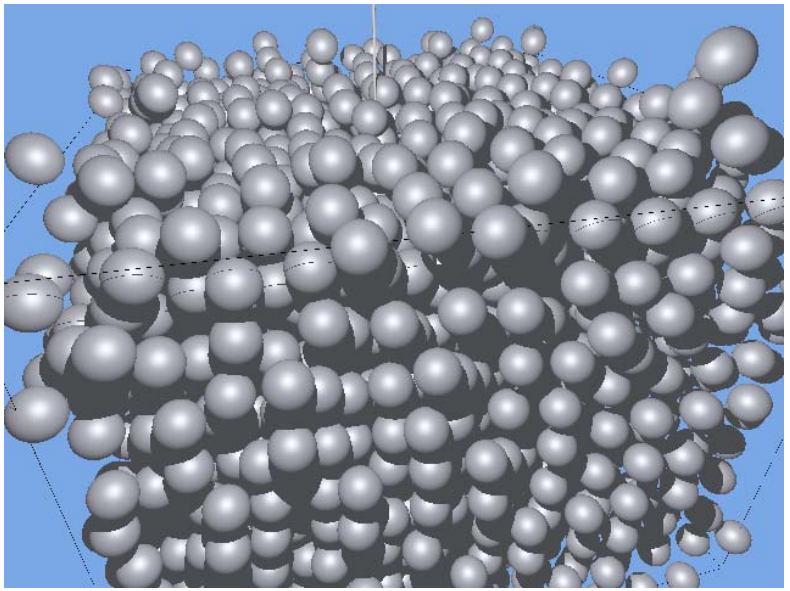
Liquid lithium simulation setup





- Temperature control is achieved by using a simple velocity scaling technique at each time step[1-3] to maintain the desired temperature at the edges of the surface.
- The resulting target surface is an amorphous liquid lithium surface 42.2 by 42.2 Å and 34.2 Å deep.

1. L. V. Woodcock, Chem. Phys. Lett. **10**, 257 (1970).
2. D. J. Evans, Mol. Phys. **37**, 1745 (1979).
3. T. Schneider and E. Stoll, Phys. Rev. B **13**, 1216 (1976).

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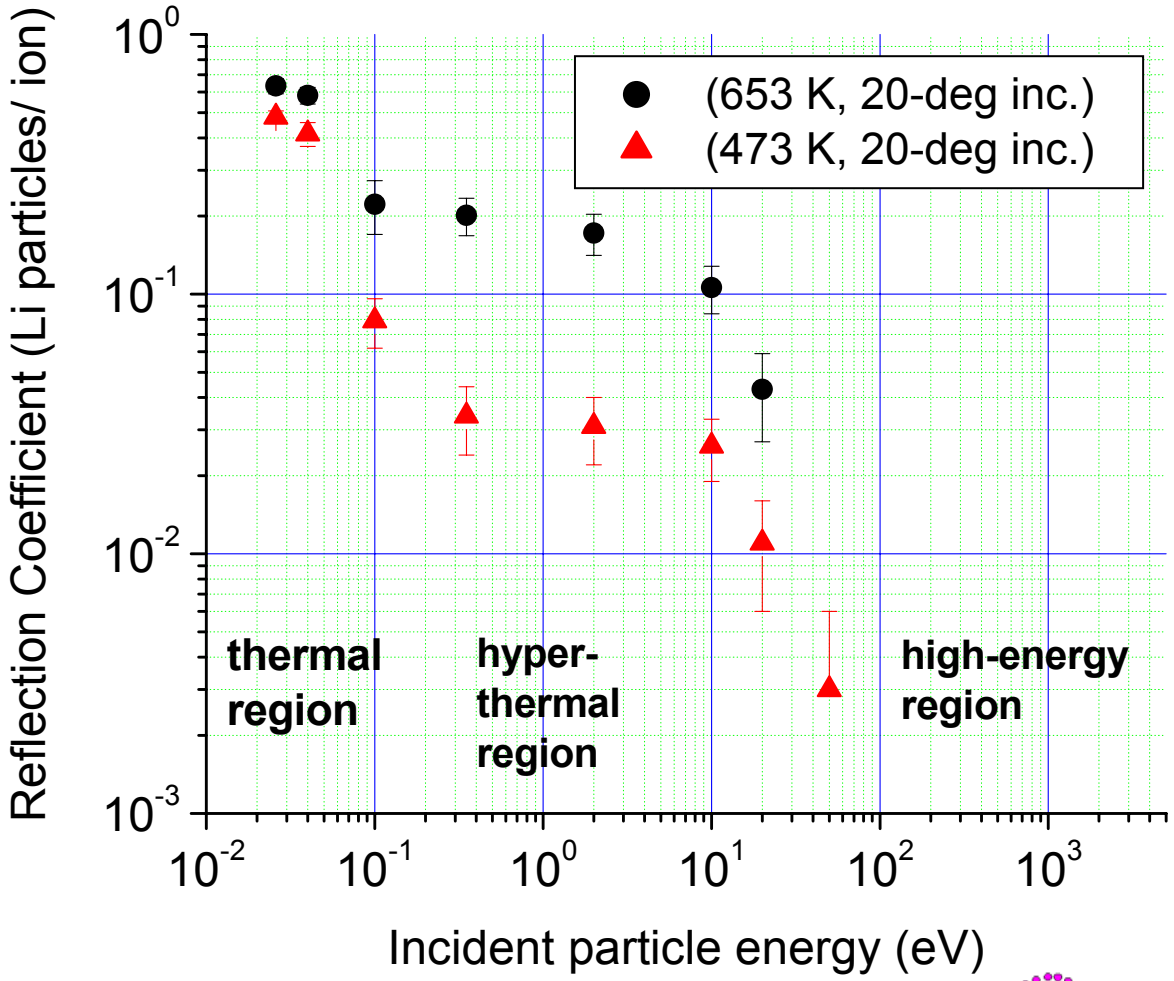
Molecular dynamics simulations of liquid lithium reflection

- NSTX cases: 473 and 653 K, 20-deg. incidence
- Reflection results show three distinct regions for low-energy self-bombardment reflection of lithium
- A region is found where the reflection coefficient varies little with incident energy (hyperthermal region)
- MD modeling continues to investigate this behavior as well as oblique bombardment (45,75-degree inc.)
- Other issues include: other temperatures and hydrogen treatment of lithium surface



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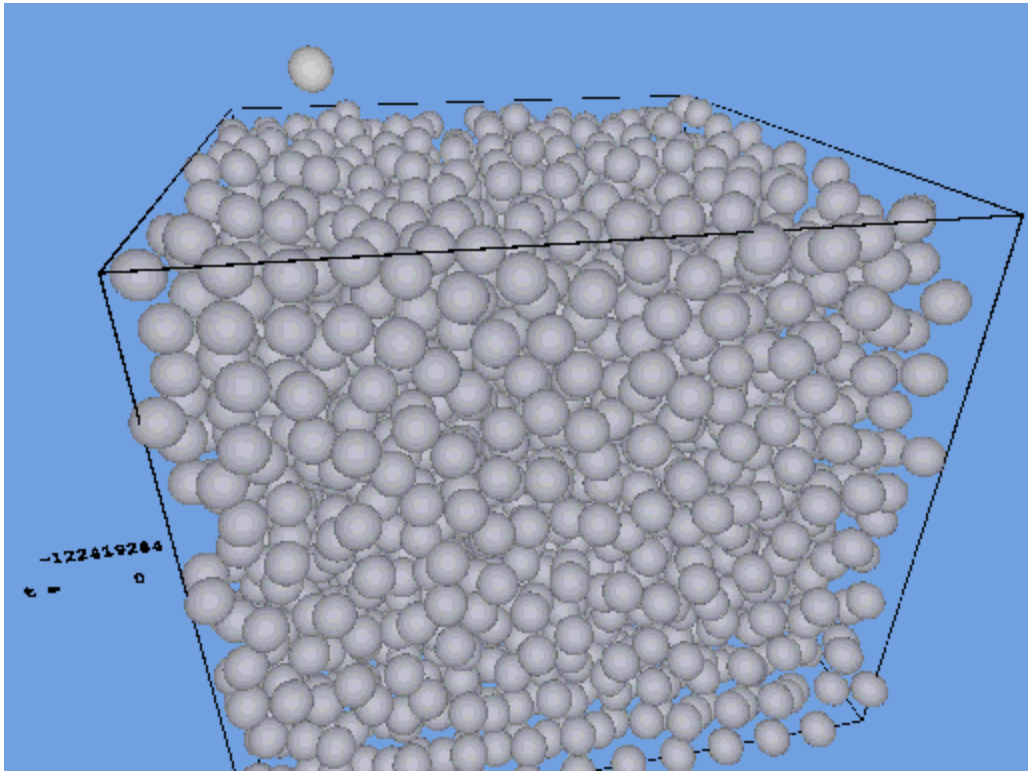
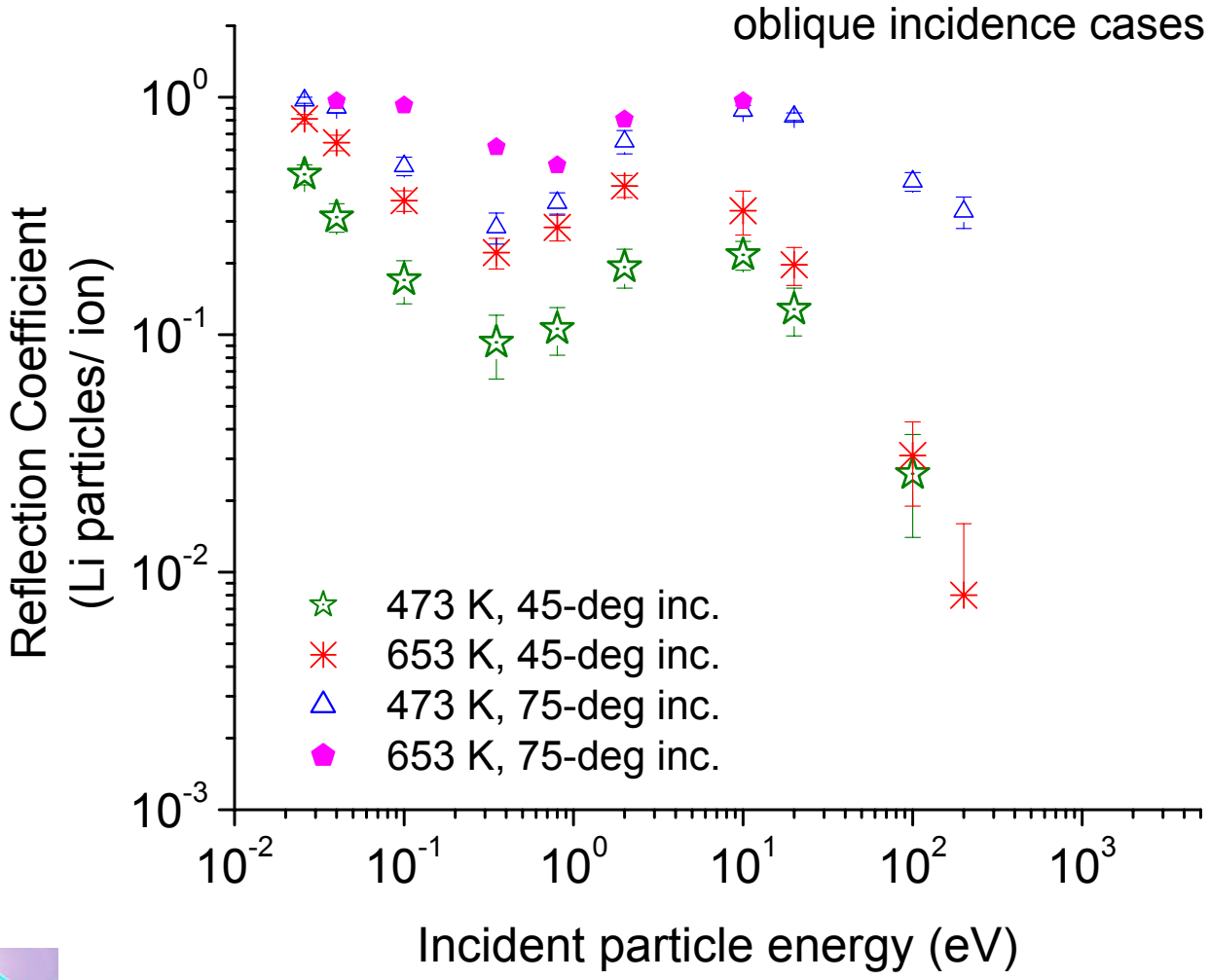
0.35 eV, 20-deg inc, 653 K



Lithium reflection at oblique incidence



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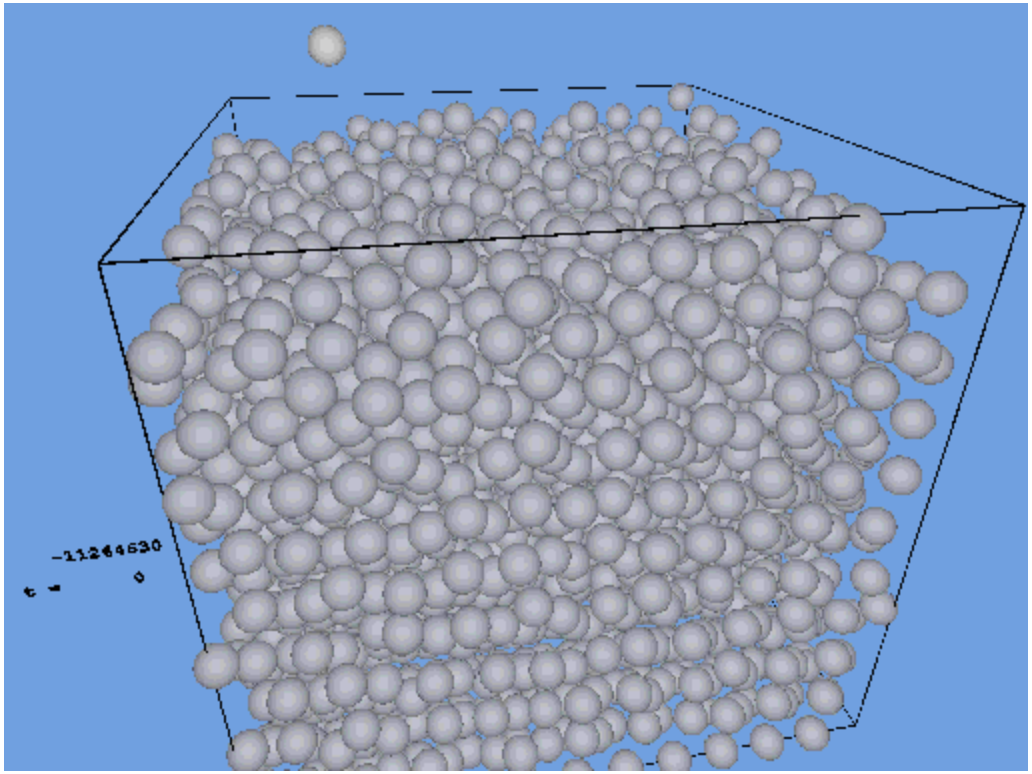
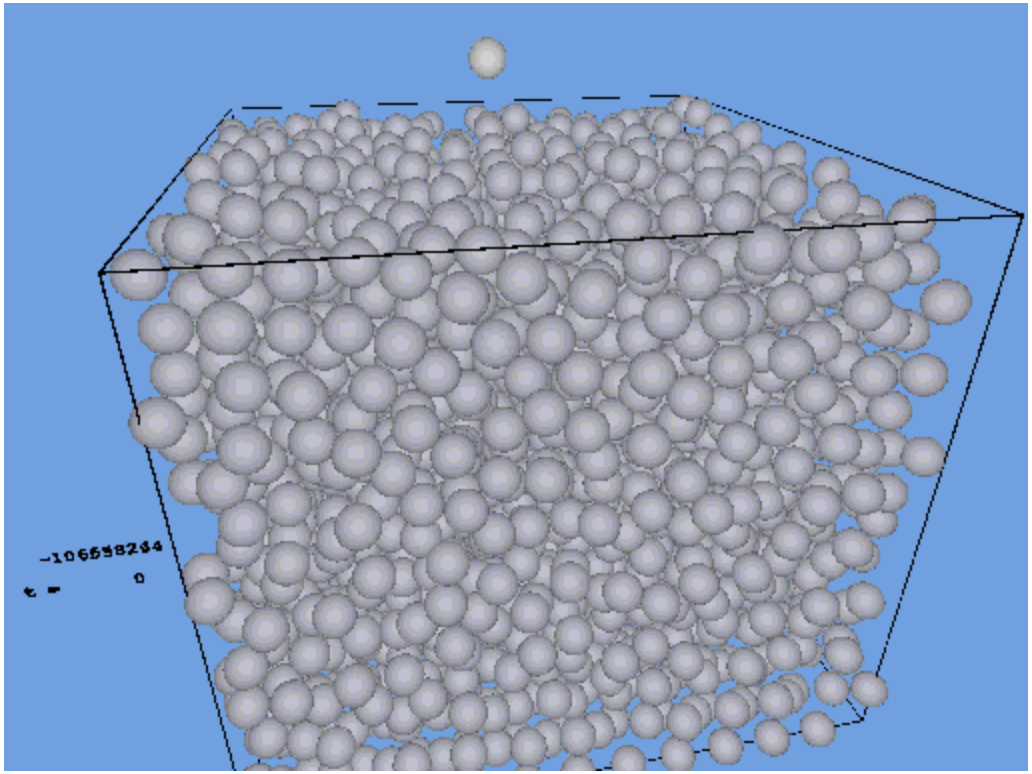
2.0 eV, 473 K at 45-deg inc.



2.0 eV, 653 K at 45-deg inc.



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MD/TRIM liquid Li erosion enhancement modeling studies

- Lithium erosion enhancement is studied using molecular dynamics of Li bombardment of liquid Li†
- Near-surface energy cascades are found from MD results for a variety of system temperatures
- The recoil energy and angular distributions are implemented in a Monte Carlo code (modified VFTRIM-3D) to obtain absolute lithium sputtering yields for comparison with experimental Li erosion data
- In addition, the surface binding energy from MD is implemented in VFTRIM-3D as a function of system temperature

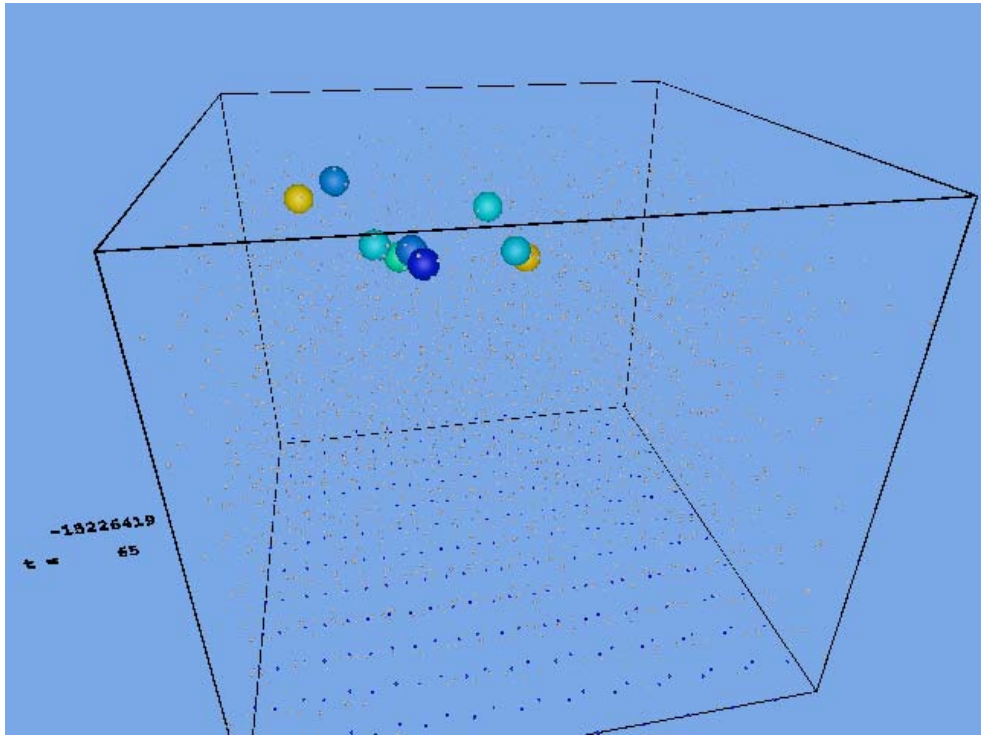

Figure shows near-surface energy cascade of recoils from a 100 eV, 45-deg. incident Li atom. Colors represent energy magnitudes (red – highest, blue - lowest). Only atoms with 10*kT or more are shown.

† L.E. Gonzalez, private communication, 2002
L.E. Gonzalez, J. Phys. Conds. Matter 5 (1993) 4283.

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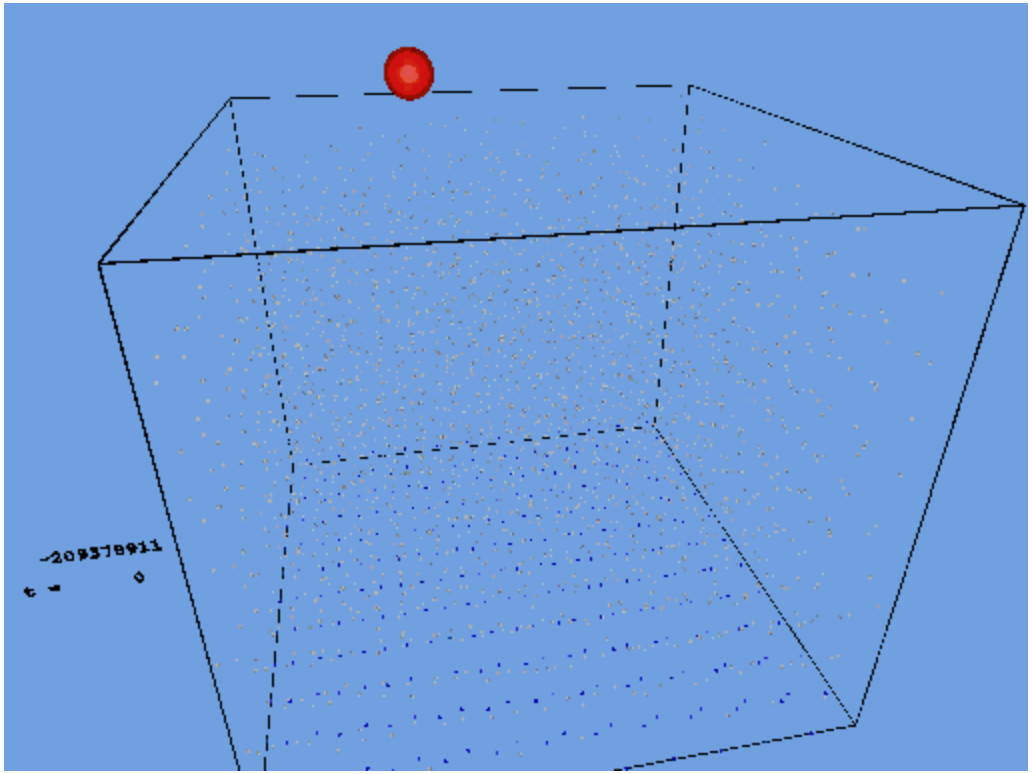
200 eV, 45-deg. Li on liquid Li, reflection and sputtering



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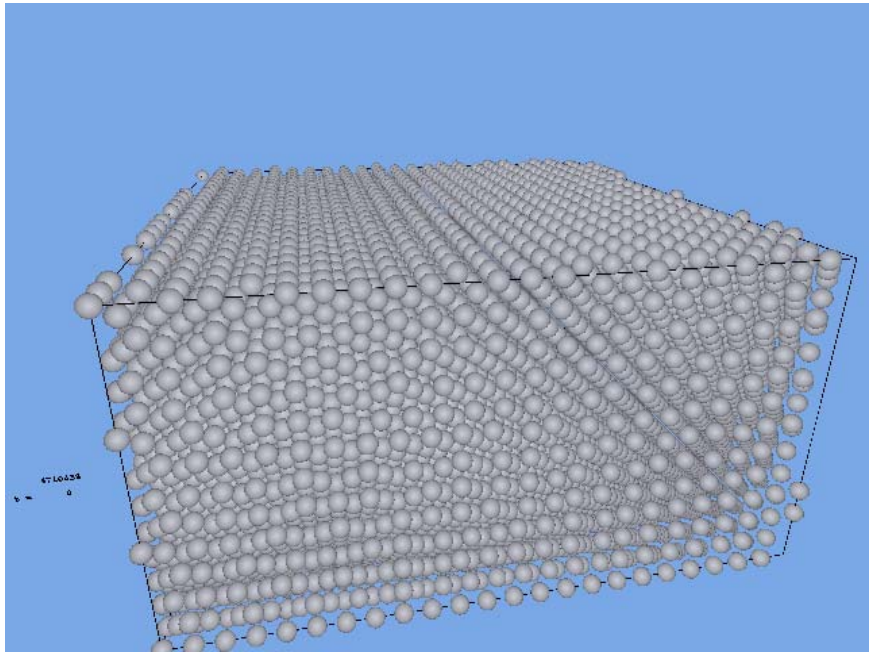
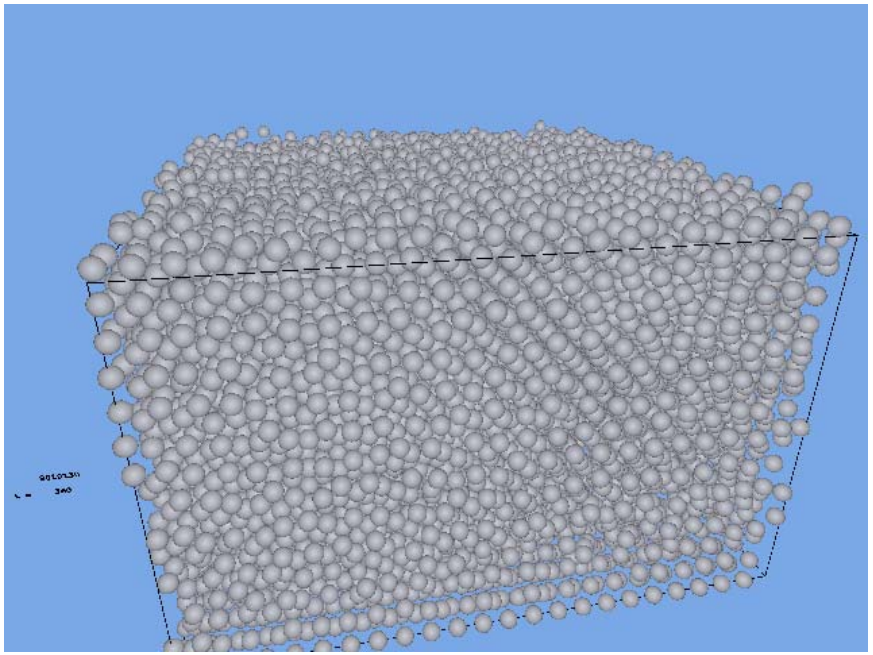
Analysis of molecular dynamics simulations of liquid surfaces





- Efforts begun in building larger lattices being mindful of computational expense.
- The size of the lattice may be relevant in modeling incident energies ranging from 300-700 eV. The effect of size on cascade dynamics are currently under investigation.
- A lithium lattice of about 13,300 lithium atoms is now in use and has been heated to temperatures of 473 and 653 K. Equilibration times ~ 25-250 picoseconds.

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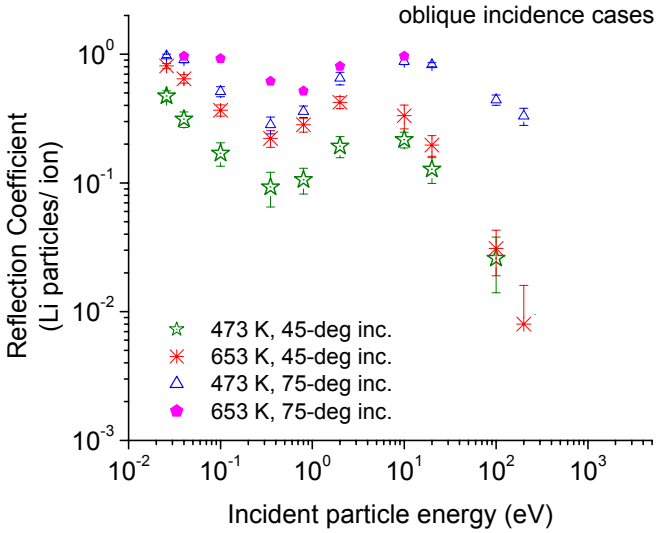
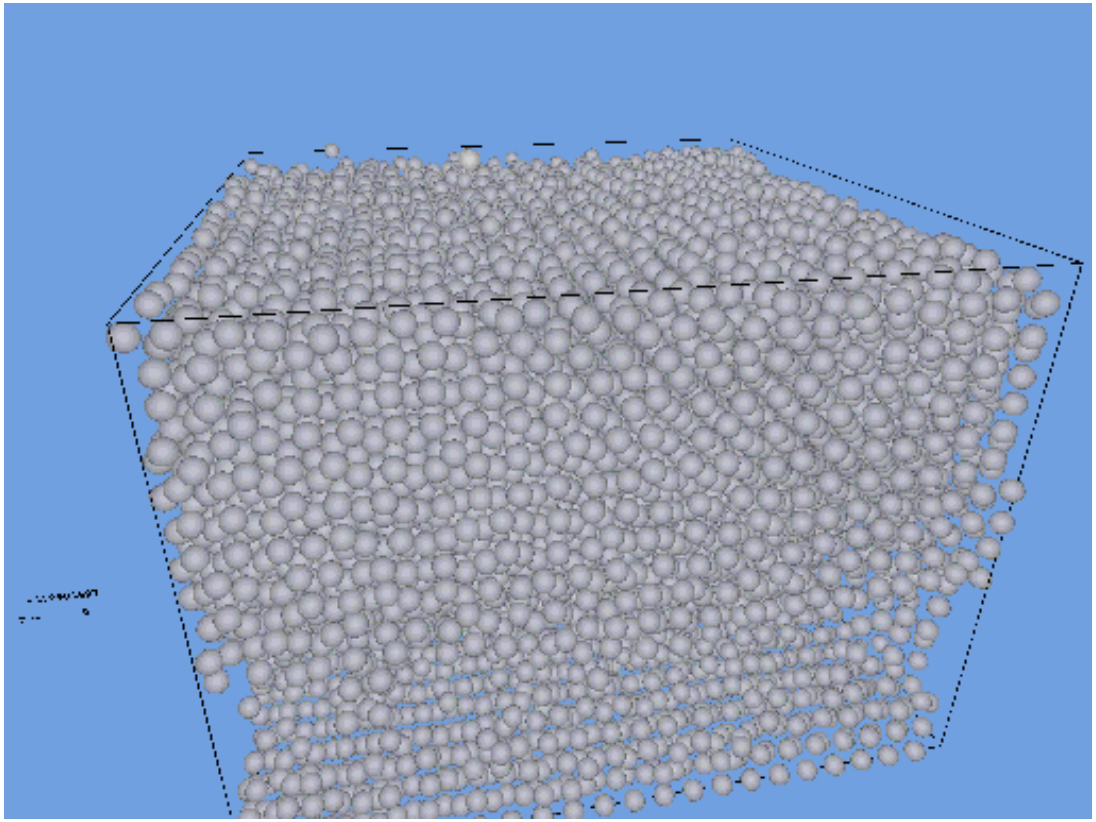
Case for reflection with large lattice: 75-deg inc. 10 eV

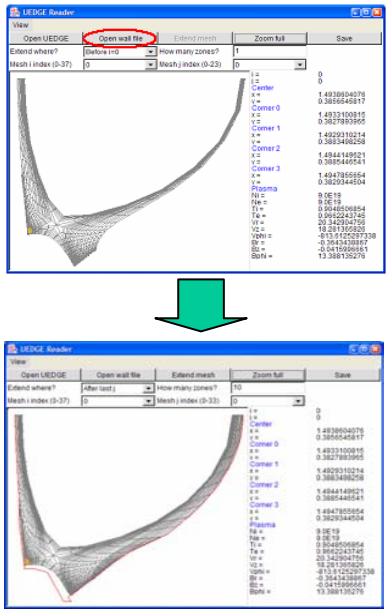




T = 473 K

NSO/FIRE Modeling

- Original model
  - UEDGE plasma solution from Rognlien/Rensink was modified
    - Mesh extended out to first wall, plasma zones filled in
    - Modeled ion flux to first wall, including diffusive and anomalous transport
      - Flux = $D \times n_i / \lambda_n$
      - $D_{perp} = D_{Bohm} = 0.06\ T_e/B$
      - $D_{anomalous} = 0.1\ m^2/s$ as in UEDGE
  - DEGAS2 used to calculate deuterium fluxes to first wall
  - Sputtering of beryllium from first wall calculated with VFTRIM-3D
  - Transport of sputtered Be to divertor calculated with WBC+
  - Results:
    - Be sputtering was low ($2.2 \times 10^{20}\ s^{-1}$)
    - Be current of $8.2 \times 10^{19}\ s^{-1}$ to inner and $2.9 \times 10^{19}\ s^{-1}$ to outer divertor plate



- Current flux model:
  - D_{perp} minimum is $0.1\ m^2/s$
  - Ion density at last UEDGE zone used (rather than at zone adjacent to wall)
  - Results:
    - Total Be sputtering increases to $4 \times 10^{20}\ s^{-1}$ (increased by about a factor of 2)
    - Be current of $1.8 \times 10^{20}\ s^{-1}$ (~ 2x) to inner and $8.4 \times 10^{19}\ s^{-1}$ (~3x) to outer divertor plate
- Beryllium flux to divertor goes to ANL for mixed material erosion analysis with the ITMC code

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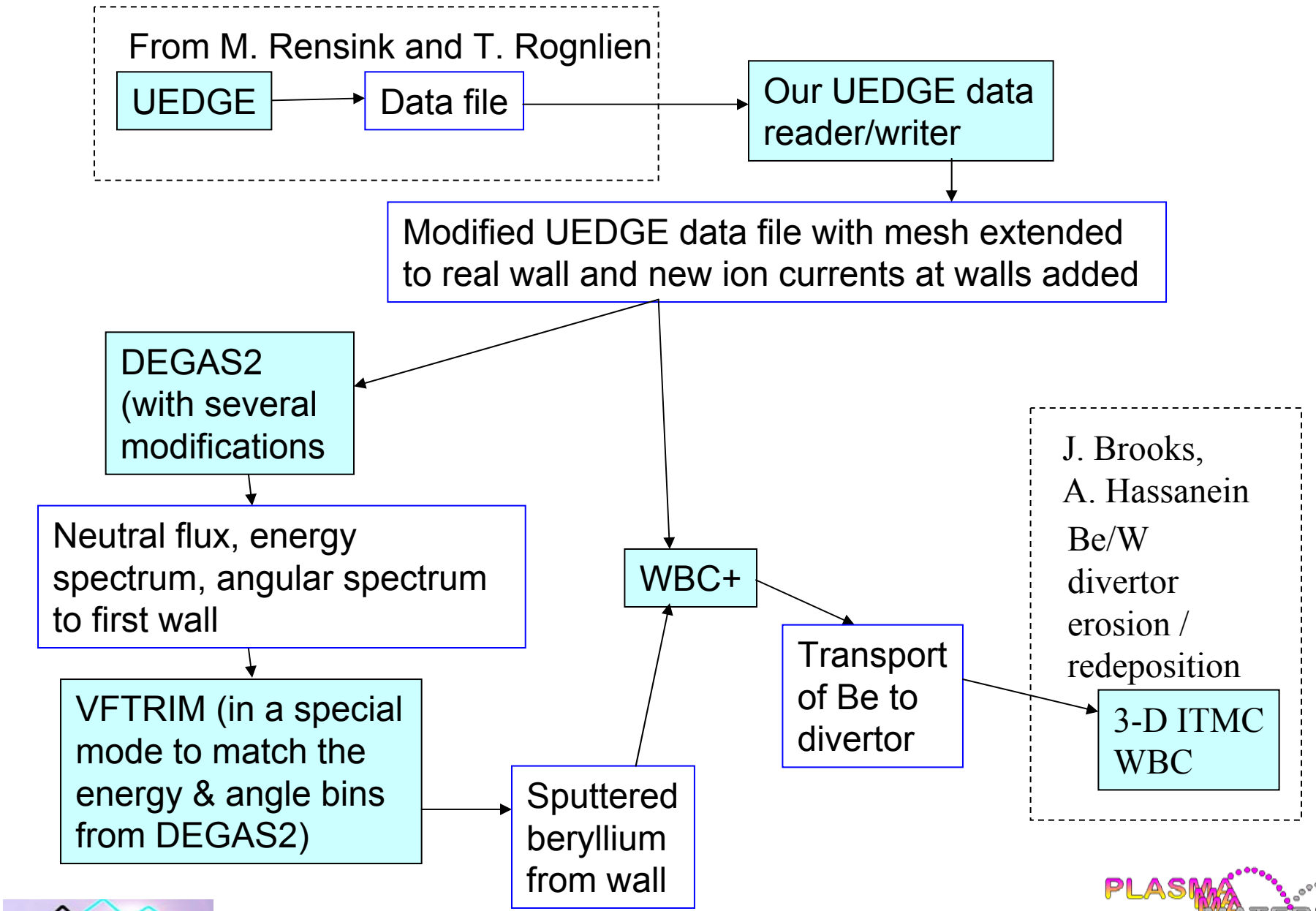
From M. Rensink and T. Rognlien
UEDGE
Data file
Our UEDGE data reader/writer
Modified UEDGE data file with mesh extended to real wall and new ion currents at walls added
DEGAS2 (with several modifications
Neutral flux, energy spectrum, angular spectrum to first wall
VFTRIM (in a special mode to match the energy & angle bins from DEGAS2)
Sputtered beryllium from wall
WBC+
Transport of Be to divertor
J. Brooks, A. Hassanein
Be/W divertor erosion / redeposition
3-D ITMC WBC

Conclusions and Future Work

- Work ongoing on reflection from “soft” and “hard” carbon surfaces
- C_3 reflects more than C_2 due to bonding nature of carbon trimer
- Reflection for low-energy Li on liquid Li shows large yields at thermal and hyperthermal energies
- The yield rises with angle of incidence, however functional behavior is different
- More work continues coupling MD simulations with TRIM in understanding nature of enhanced erosion of liquid Li (in particular) or liquid-metals (in general)…more in tomorrow’s talks: Allain and Ruzic
- Li particles that reflect at thermal or hyperthermal energies will mostly consist of neutrals
- Be currents of the order of 10^{20} s^{-1} reach the inner and outer divertor of FIRE